Quantum Design

MPMS Application Note 1014-203

Outline of Data Regression Routines

The magnetic moment of a sample is measured by moving the sample through the detection coils in a series of discrete steps. At each of these steps, the sample's magnetic moment produces some magnetic flux through the superconducting detection coils, which is then detected by the SQUID. A feedback circuit counteracts the flux contribution from the sample by introducing an opposing magnetic field to the superconducting circuit. Measuring the current this feedback circuit produces is the basic data that the MPMS treats as the signal from the sample. The feedback current produces the voltage associated with the signal of a sample as it passes through a known resistor. A voltage is recorded at each of the sample positions. To reduce random noise, each of these measured voltages is an average value of many (1 to 30,000) measurements taken at each sample position.

The software stores each measured voltage as well as other data in a matrix. The other data in the matrix is dependent on whether linear or iterative regression is used. Two corrections, demeaning and detrending the data, are performed on the measure signal before it is compared to the ideal signal. In this way, the raw data resemble the ideal signal. The full scan makes no attempt to idealize the sample. The longitudinal SQUID calibration factor is used to convert the measured voltage to a magnetic moment. A graph (see **Figure 1**) is provided to correlate these parameters to the ideal signal.

Data Matrix

The software now has a series of voltages from which a value of the magnetic moment is determined. In order to compare the measured signal to an ideal signal and to allow for various corrections, the software stores much of the relevant information in a matrix.

One column of the matrix calculates the ideal dipole signal from basic magnetic theory. The other two to three columns hold information necessary to compensate for offsets and drifts. Each row of the matrix has either three or four entries corresponding to a single voltage measurement with the exact number of entries depending on whether the linear or iterative regression is used.

For a linear regression, three parameters are fit to the data set. These parameters correspond to a constant offset, the slope of the linear drift, and the amplitude of the dipole signal. The iterative regression has these three parameters and an additional parameter that represents a small correction to the sample position. The value of these parameters is allowed to vary, modifying the characteristics of the ideal dipole signal, until the difference between the measured data and the ideal signal drops below some threshold.

Demean the Data

Although the MPMS has been designed to optimize its data acquisition, the measured data points are the superposition of the signal from the sample with undesirable noise and machine drifts. The first correction is the removal of a constant offset, or demeaning the data. The offset is calculated by determining the average value of the data set. To demean the data, each data point has this average value subtracted from it. The resultant data set has the same shape, but the whole plot is shifted up or down by a constant amount, and the average value of the signal will be zero. Without this, it would be possible for the measured data to have exactly the same shape as the ideal signal except for a large constant offset. Due to the large difference between the two curves, the software would judge the two curves as very different, and the magnetic moment would not be calculated.

Detrend the Data

Next, the data is detrended, meaning a linear drift is subtracted. The detrend program takes the data set and fits a line that best fits it using a chi-squared algorithm. This drift contribution is calculated and subtracted from each data point. The result of these steps is a series of data points that are assumed to be the voltages due to a perfect dipole. At this point, one of the three algorithms to calculate the amplitude of the voltage signal operates on the measured data points. This is discussed in the *Scan Types* section below.

Longitudinal SQUID Calibration Factor

The relation between the measured amplitude of the signal and the actual magnetic moment is different for each unit and is accounted for by the longitudinal SQUID calibration factor. Palladium is used to determine this calibration factor because its magnetic moment is easy to calculate. Essentially, the calibration factor is calculated by dividing the amplitude of the measured voltage signal by the known magnetic moment of the palladium sample. This scaling factor is used in all measurements to convert the measured voltage back to a magnetic moment.

Scan Types

The three methods of scanning the sample determine the resultant measurements with unique parameters. The scan types are full scan, linear regression, and iterative regression.

Full Scan

The full scan is the least involved of the three algorithms. It does not attempt to check that the signal looks anything like the dipole that is expected and makes no corrections for poorly centered samples. This algorithm just takes a root mean square of the sum of the voltages and scales it to get an emu value. Mathematically, this is

$$\text{EMU} = \frac{\text{Range}}{\text{Gain} * \text{SQUID Calibration Factor}} \sqrt{\Sigma v_i^2}$$

The full scan algorithm does not analyze very small signals as effectively as the iterative regression and linear regression algorithms. It is generally used as the initial procedure in locating a sample's center position in a full centering measurement.

Linear Regression

As mentioned earlier, the linear regression algorithm has three variable parameters that modify the ideal dipole signal. They represent a constant offset, the slope of the linear drift, and the magnitude of the amplitude of the voltage signal. The previous demeaning and detrending of the measured data ensures that the linear regression's offset and linear corrections will be relatively small. This is an important factor for the iterative algorithm to work successfully.

The algorithm initially starts with a best guess for the values of the three parameters. Using these values, the software modifies the ideal dipole signal. It then computes the difference between the measured data and the modified signal. If the difference is below a predetermined threshold, the amplitude of the ideal dipole signal is used to calculate the magnetic moment. If the difference between the data sets is larger than the threshold, the parameters are adjusted, the ideal signal is modified by these new parameters, and the whole process is repeated.

Iterative Regression

The iterative scan is similar to the linear scan in that it varies several parameters that modify the ideal dipole signal. The iterative algorithm has the same three parameters as the linear scan and an additional parameter that makes a correction for a sample that may not be perfectly centered. This correction represents the effect of small disturbances in the position. Mathematically, if $M(z_0)$ represents the signal of an ideal dipole at the vertical position z and five is a small displacement from this position, the signal can be expressed as

$$M(z_0 + \delta) \equiv M(z_0) + \delta \frac{M(z_0)}{\delta z} * \delta$$

From a computational point of view, it is much more efficient to treat this variation as a small additional contribution to the signal, rather than to add the displacement to the position and recalculate the new signal. So, as parameter δ is varied, the effective position of the sample moves, and the measured data is compared to the ideal data as before. The maximum value of δ is ± 5 mm.

The software performs the same calculations and follows the same procedures for the iterative regression as it does in the linear regression. Iterative regression cannot locate the signal if the signal is beyond a certain tolerance. The linear regression algorithm is substituted for the iterative regression algorithm if the center cannot be found.

Graph

The following graph shows the effects of the demean and detrend routines. The line labeled "drifted.dat" is an ideal dipole signal with a constant offset and linear drift added. The plot labeled "demeaned" is the drifted data after the demean algorithm has operated

on the data. Similarly, the plot labeled "detrend" shows the drifted data after both demean and detrend have acted on the data. The plot labeled "ideal" is the ideal dipole signal that had the drift added to it.
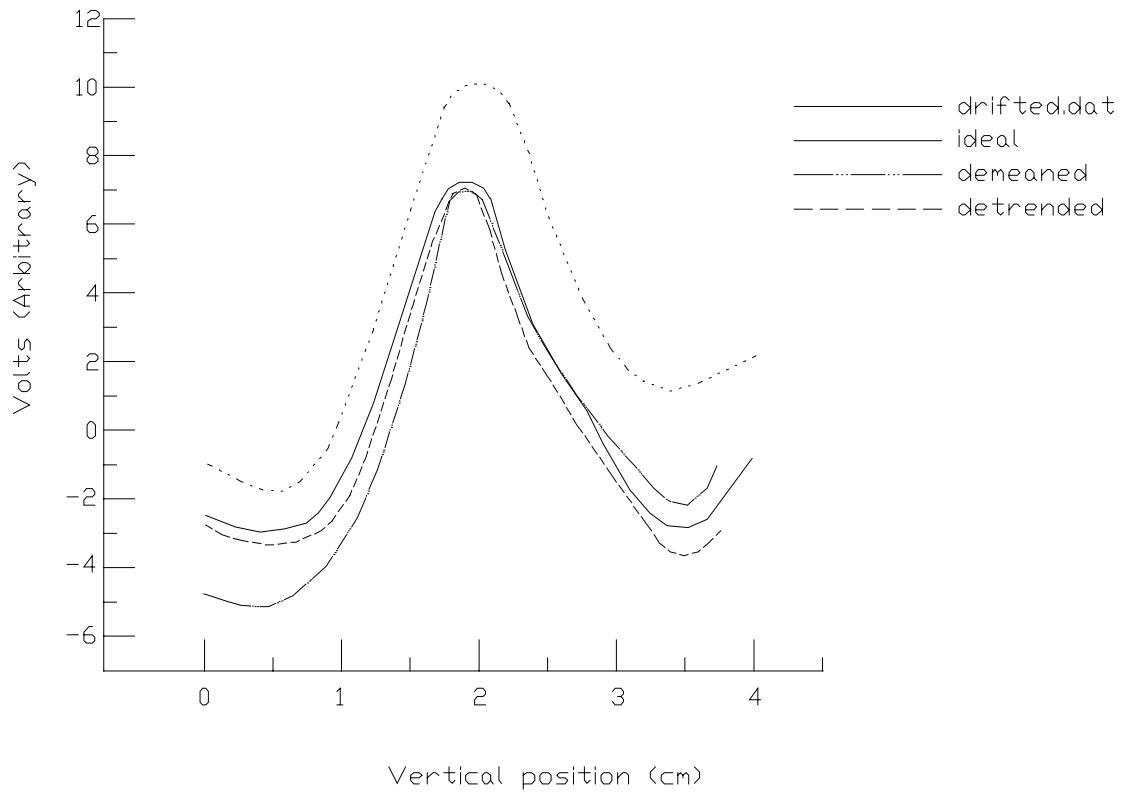
Figure 1. Effects of the demean and detrend routines.